PROJECT NUMBER: 2500
PROJECT TITLE: Fundamental Chemistry
PROJECT LEADER: J. I. Seeman
PERIOD COVERED: November 1989

I. **INORGANICS AS NOVEL TOBACCO MATERIALS ADDITIVES** (Fournier, Kallianos, Paine, Podraza, Seeman)

A. **Objective**: To develop inorganic materials for novel applications for reduced sidestream, for burn-rate modification, and enhanced subjectives in cigarettes and for required properties in novel smoking materials.

B. **Results and Plans**: Work continues on sol-gel derived $MgCO_3$ particles: new samples were prepared, submitted for handsheet-making, the effects of drying/heating conditions on particle size were investigated (BET 236 m^2/g after heating to 450°), and dynamic light scattering was performed on the sol (average particle size of 118 nm). Zirconia gels coated (5%) on cigarette paper were not effective in the burn-rate test while the zirconia-acetylacetonate complex was effective.

Optimization of the magnesite ($MgCO_3$) preparation continues. To date, magnesite hydrothermally prepared from hydromagnesite ($Mg_5(CO_3)_4(OH)_2.5H_2O$) at 250°C for 14 hours has given the smallest particle size as determined by laser diffraction. Shorter periods of time result in the incomplete conversion. Approximately 70 g of magnesite prepared under the aforementioned conditions will be available this week for paper making.

Nesquehonite ($MgCO_3.3H_2O$), was prepared by adding magnesium chloride to a stirred and sonicated solution of potassium bicarbonate. Attempts to prepare nesquehonite without the use of sonication resulted in a mixture of $KHCO_3.MgCO_3.4H_2O$ and nesquehonite as confirmed by x-ray diffraction. This is a case where sonication aided the reaction. The retention of the nesquehonite in paper was low and papers were not made. It may find use as a coating.

A K/Fe phosphate was prepared hydrothermally. X-ray diffraction results to determine the actual phase are pending.

II. **REMOVAL OF NICOTINE FROM AQUEOUS TOBACCO PROCESSING FLUIDS** (Paine, Secor, Seeman)

A. **Objective**: To develop techniques to remove selectively nicotine and other alkaloids from aqueous tobacco processing fluids.

B. **Results and Plans**: Development of data necessary to develop a pilot plant scale clay-mediated nicotine separation scheme is in full progress. Various clays are being examined, and the quantities of nicotine absorbed, sulfuric acid need to reextract the nicotine, and water washes are being determined. Clay

lifetimes (i.e., recycle capabilities) are also being examined. In collaboration with A. Kumar, specialized equipment for back flow extractions have been designed and assembled. Various processes are being considered for potential commercialization, and interactions with outside vendors/consultants have been valuable.

III. **NICOTINE DESTRUCTION** (Podraza, Secor, Seeman)

A. **Objective**: To develop a commercial scale procedure for the chemical destruction of nicotine.

B. **Results and Plans**: Experimental studies on three nicotine destruction procedures have been very carefully examined, and work is nearly completed: hydrogen peroxide, sodium hypochlorite, and ozone. In conjunction with A. Frisch, U-^{14}C-nicotine has been used to follow mass balance in these three procedures, and in all cases, >98% carbon has been accounted for. The major and most of the minor products in the three methods have been identified, and some optimization in reaction conditions have been successfully performed. A full report is being written and patent disclosures are being prepared.

IV. **FLAVOR/ODOR CHEMISTRY** (Howe, Paine)

A. **Objective**: To prepare new substances for flavor/odor evaluation.

B. **Results and Plans**: In support of Y. Houminer's vanillin program, ca. 10 g of a vanillin release compound was prepared under a high priority-rush request by a novel route and transferred to Flavor Development.

V. **MISCELLANEOUS** (Secor)

Results: 2-(2-Hydroxyethyl)quinoline was prepared and sent to E. Bernstein as a model for the flavor release systems being developed for a variety of flavor objectives. Two 2,4-dinitrophenylhydrazones (of formaldehyde and acetaldehyde) were prepared for R. Comes as standards in the SS program.